

• USANS Data Reduction

10/2001 Vers. 1

This implementation of the USANS data reduction procedures is designed to allow reduction of raw (ICP) scans from the BT5 USANS instrument into standard I(Q) format. Data output is smeared with the resolution function of the USANS instrument, so called "slit-smeared" data. This reduction package currently does not desmear datasets.

The USANS Reduction macros are designed to provide an easy to use, graphical interface for the reduction of raw data files into a portable ASCII format. The USANS macros and all raw ".bt5" data can be easily copied and carried to your home institution for convenient use. As of 10/2001, USANS Reduction macros require IGOR Pro v. 4.0x. As always, the macros will work with the free Demo version of IGOR.

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Overview of USANS

In general, a complete USANS measurement will require sample and empty cell scattering measurements as well as a background countrate. Scattering measurements are typically broken into several files, each covering separate non-overlapping angular ranges (q-range). Since the intensity is measured across the central beam for both sample and empty cell scattering measurements, transmission information is implicitly included.

As data is collected during a USANS experiment, a copy of your data is mirrored to a central server, "Charlotte". This server is available through guest connections to PC's through the Network Neighborhood, and to Macs through AppleShare. This allows you to reduce your data from any location within the building. Your data will be located in a folder on Charlotte->ICP Data->bt5->yyyymm->month. "yyyymm" is the year and month of the beginning of the reactor cycle, and "month" is the month of data collection. The original data file remains on the instrument control computer as a backup. Raw ICP data files collected on USANS are denoted with the extension ".bt5". Data files are ASCII text containing header information followed by raw detector count values versus analyzer angle.

Data reduction procedures automatically detect the zero angle peak of the main beam, convert the angle into q ($1/\text{\AA}$), and normalize to monitor counts and counting time. The transmission as measured by the analyzer (T_{Rock}) is determined by measuring the peak intensity with and without the sample: $T_{\text{Rock}} = I(\text{peak})_{\text{sample}} / I(\text{peak})_{\text{empty}}$. The transmission measured by the transmission detector is calculated again from the ratio of counts with and without the sample, this time with the analyzer detuned (angles greater than 2°). $T_{\text{Wide}} = \text{TRANS}_{\text{sample}} / \text{TRANS}_{\text{empty}}$. Wide angles are used since the transmission detector countrate is attenuated at analyzer angles close to the main peak.

Data correction is made using the following relation:

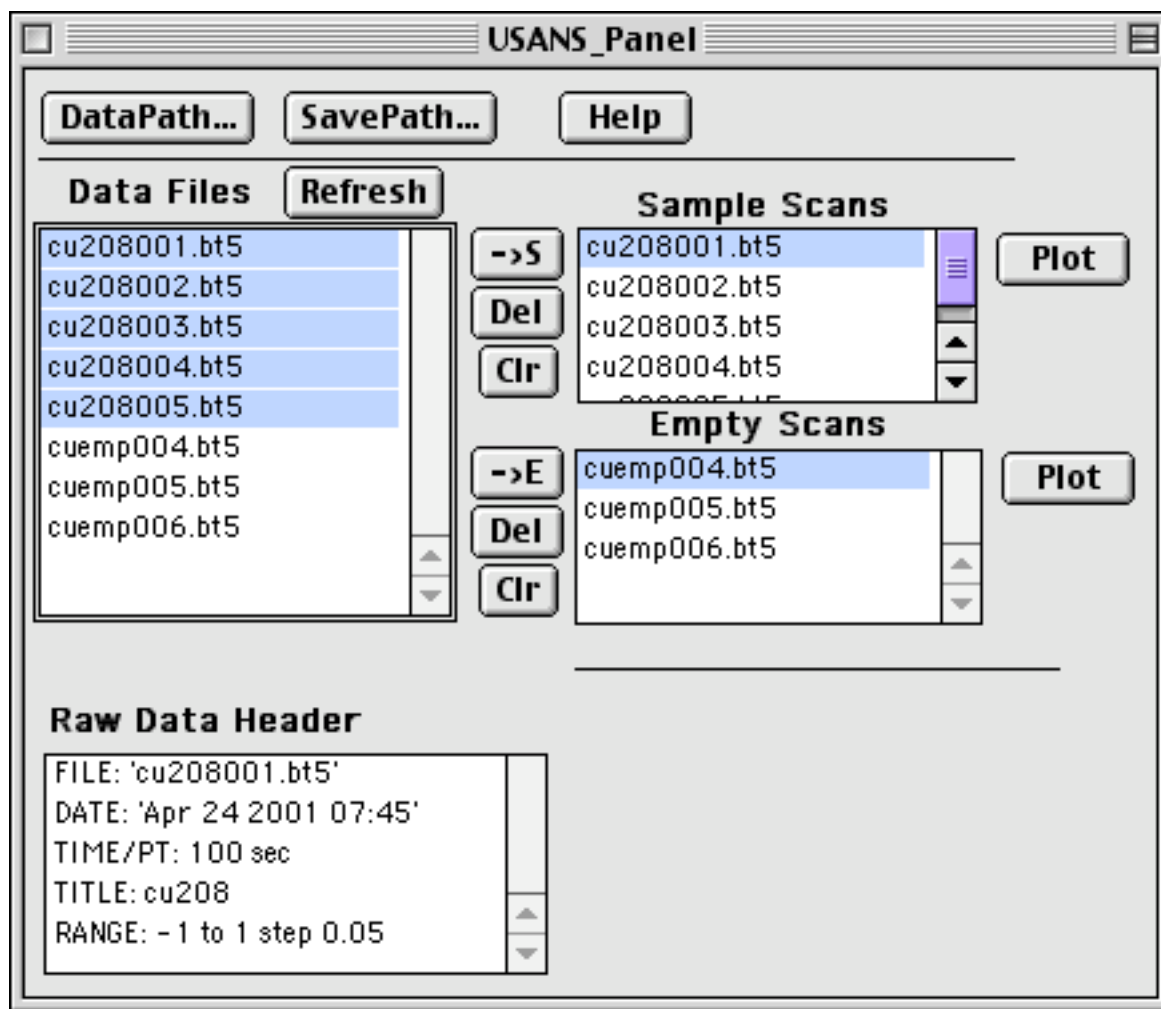
$$I_{\text{COR}}(q) = I_{\text{SAM}}(q) - T_{\text{Rock}} I_{\text{EMP}}(q) - (1 - T_{\text{Rock}}) I_{\text{BGD}}$$

Corrected data is converted to absolute scale by a conversion factor:

$$K = 1 / [I_{\text{peak}} T_{\text{Wide}} d_s \Omega]$$

where d_s is the sample thickness in cm, and $\Omega = 2.7\text{E-}7$ ster is the solid angle accepted by the analyzer.

Main USANS Controls



The USANS_Panel will open automatically when a blank reduction template is opened. Initially all of the list boxes will appear empty, and are waiting for data.

The controls on the panel are:

DataPath...: Use this button to select the folder containing the raw ICP data files. This is typically the file server "Charlotte", in the correct subfolder of Charlotte:ICPData:BT5:

SavePath...: Use this button to select the folder on your local computer where

corrected data is to be saved.

Help: Displays this USANS Data Reduction help file.

Refresh: Refreshes the file list from the folder chosen in "DataPath"

->S: Transfers the selected raw data files to the list of Sample files. Does nothing more than copy the filenames.

->E: Same action as "->S", but adds to the list of Empty files.

Del: Deletes the selected file from the Sample (or Empty) file list, whichever list is adjacent to the button.

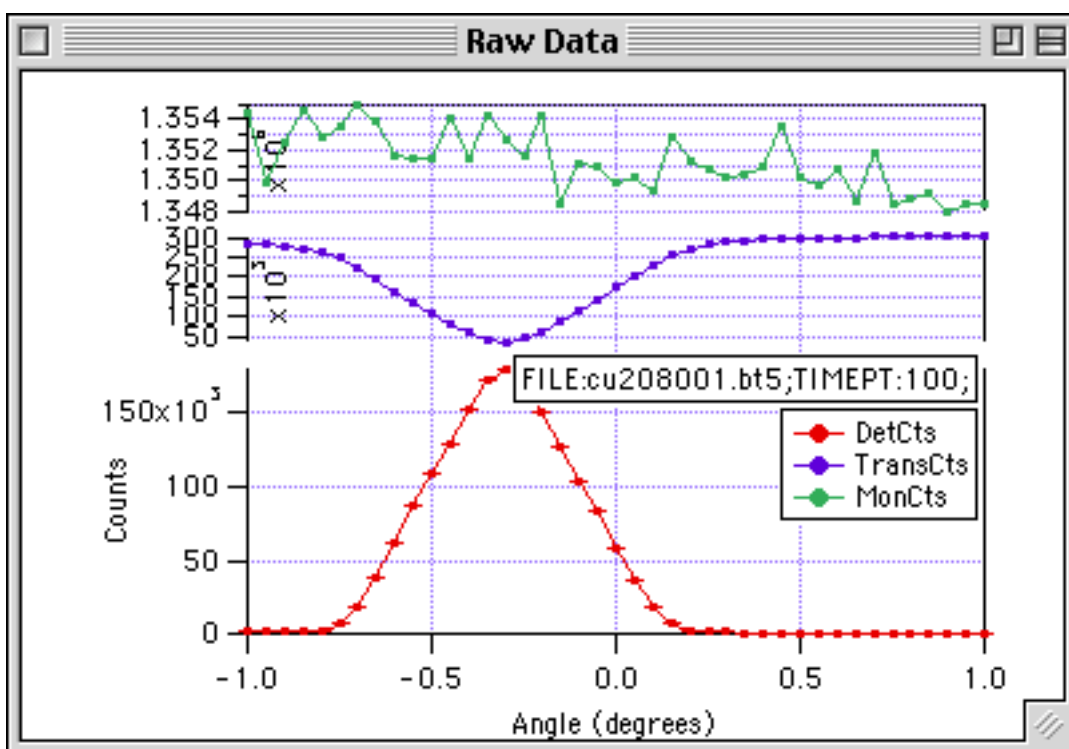
Clr: Clears all entries from the Sample or Empty files list, whichever list is adjacent to the button. This also clears SAM or EMP data from the COR_Graph, and clears COR data if necessary.

Plot: Plots the Sample or Empty files in the COR_Graph window. Before plotting the raw data, the zero angle is located, data sets are combined and normalized, and angle is converted to q-values ($1/\lambda$).

- The raw data file list is limited to include only files whose name ends in ".bt5" indicating that they are raw USANS data files. Do not change the extensions of your raw data files, and do not use a ".bt5" suffix on your corrected datasets.
- The Raw Data Header automatically displays the header information of the selected raw data file. Filename, date/time of collection, sample title, counting time per point, and the angular range/step are listed. If there are multiple files selected, the header of the first file is displayed.
- A graph of the selected [Raw USANS Data](#) file is automatically plotted when a file is selected. The graph is automatically updated when a new file is selected.
- The Sample file list and the Empty file list do not need to have runs added in angular order. Files in the list will be combined and sorted by detector angle.
- There is a short sentence of help explanation associated with each button or control on the USANS_Panel and the COR_Graph. On windows, this text is displayed at the bottom of the screen when the mouse is over the control. On the Macintosh, text is displayed by balloon help, which can momentarily be activated by holding down ctrl-opt-cmd.

Raw USANS Data

Selecting a raw data file produces a graph similar to the following:

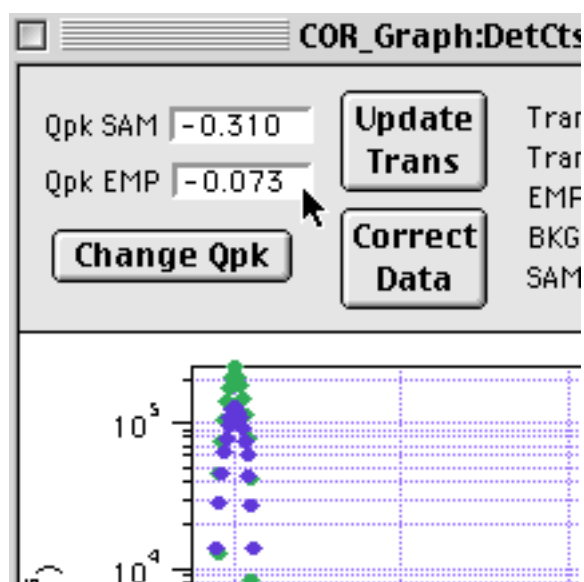


The three traces displayed are (top-to-bottom): Monitor Counts, Transmission detector counts, and Main Detector counts. Count values are not normalized and the error bar shown is due to counting statistics. Counts are plotted against the angle of the analyzer. This plot is useful for inspecting the contents and quality of a raw data file. It is automatically updated when a new raw data file is selected.

USANS Data Correction

Once you have identified the correct datasets for sample and empty scans by inspecting the file headers and the raw data, the following steps will guide you through the basics of reducing USANS data to a final $I(q)$ format.

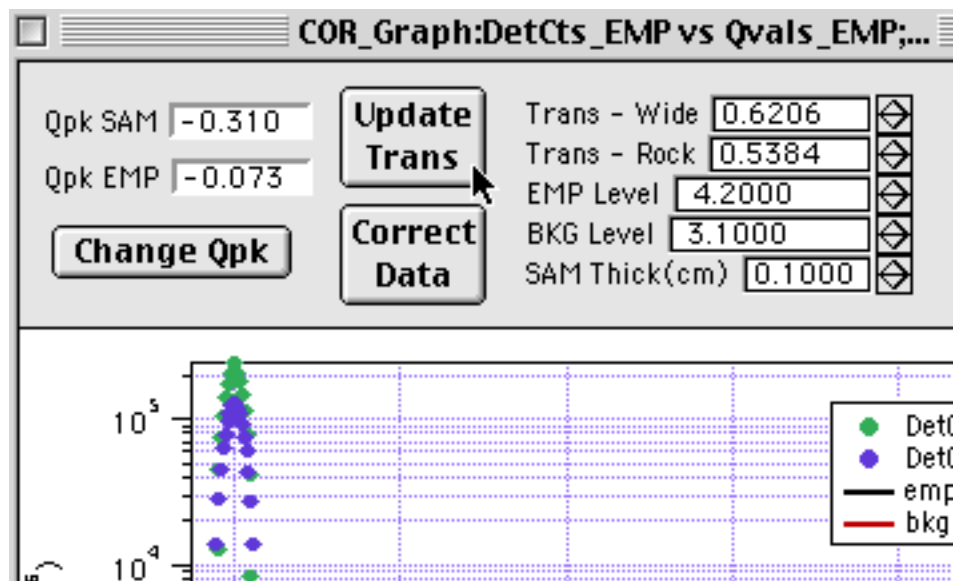
1) "Plot"-ing sample scans or empty scans will generate a "COR_Graph" window. During this step, the data is normalized to $1.0E6$ monitor counts, shifted to zero angle, and converted to Q -values. The zero angle value for each dataset is found automatically, and is reported in the upper left of the control bar. Confirm that these values make sense, and that the peaks of the scattering data are correctly at zero Q on the graph. The automatically determined peak values rarely need to be adjusted.



If peak of either file is not correct, inspect the raw data (See [Raw USANS Data](#)) to manually find a better peak position, and enter it manually by selecting "Change Qpk". You will be presented with the following dialog to change one of the peak angles. If both are incorrect, you will have to perform this operation twice.

The screenshot shows a dialog box titled "Override the peak angle". It has a "Select Data Set" dropdown menu with "SAM" selected. Below this is a text input field labeled "Enter new peak ANGLE, in Degrees" which contains the value "0". At the bottom of the dialog are three buttons: "Cancel", "Continue", and "Help".

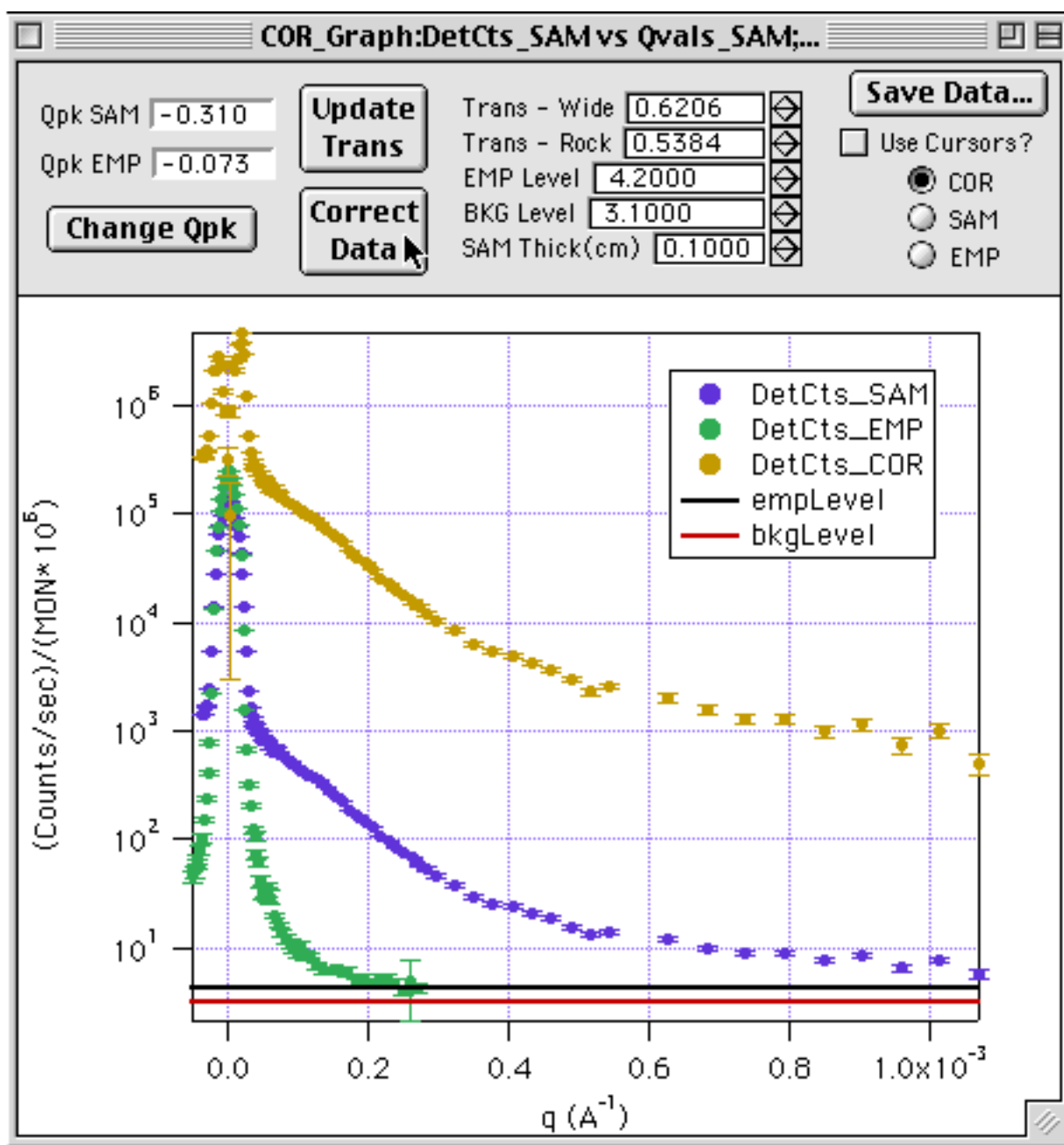
2) Once the peak locations are satisfactory, calculate both the wide angle and peak transmissions by selecting "Update Trans". The calculated values are displayed to the right of the button. Make sure that the values are as expected. Updating the transmissions has no effect on the appearance of the graph.



3) A high-Q empty cell level and constant background level will be subtracted from your data. Both levels are in detector counts per 1.0E6 monitor counts. New values can be entered directly into the fields or incremented using the arrows. The empty level will be used as an extension of the empty cell scattering data, which falls quickly to a constant level and so is typically not measured over the full q-range. The EMP level that you set will only be used where there is no experimental data. The background (BKG) level is constant throughout the entire q-range. See your local contact for the appropriate background level to use.

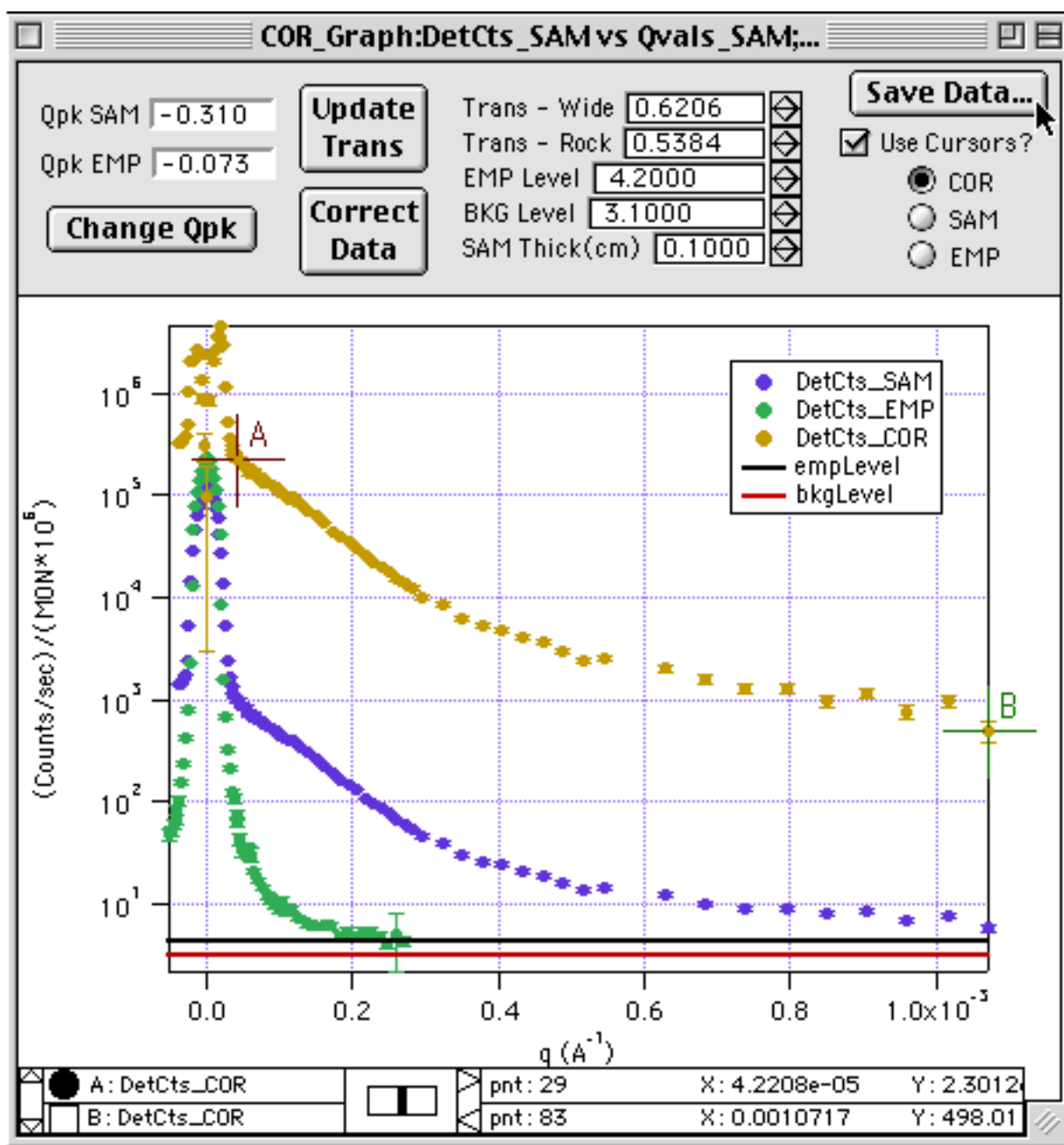
4) Enter the correct sample thickness in the field provided. This value will be used when placing your corrected data on absolute scale.

5) Now correct your data by selecting "Correct Data". A new "DetCts_COR" dataset will be generated and added to the graph. The "COR" data is on absolute scale. The EMP and SAM data have only been rescaled for time and monitor counts.



Saving USANS Data

Any of the three datasets can be saved in ASCII format by selecting the set using the radio buttons, and then "Save Data..." Sub-ranges can be selected by using the cursors (A<B) on the selected set. The active cursor can be moved L-R using the arrow keys. The active cursor is filled black in the information panel at the bottom of the graph. Clicking the circle or the square will toggle the cursor state active/fixed. The data point number, x, and y values are also shown here.



Saved data files can be loaded and plotted using the "Load_QIS_Data" under the Macros menu. This macro will also load standard SANS data files for comparison.

Desmearing USANS Data

At this time, desmearing is not performed within these data reduction macros. See your local contact for more information about desmearing your datasets.